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A Technique For The Evaluation Of Double Excitation Of Atoms By Fast Protons And Antiprotons

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A technique for evaluating cross sections for two-electron excitation in collisions of atoms with fast particles of charge Z_p is presented. The atomic wave function is approximated by a sum of pair products of one-electron wave functions, with the coefficients chosen by diagonalizing the fully correlated two-electron Hamiltonian. Thus spatial correlation is included in both the asymptotic and scattering regions by using these configuration-interaction (CI) wave functions for initial, intermediate, and final states. Use of CI wave function also allows the first-order contributions to be expressed in closed, analytical form. Both the energy-conserving and energy-nonconserving parts of the second-order amplitude are evaluated. The former (a correlated generalization of the independent-electron approximation) is analytical and the latter is a one-dimensional integral. In helium it is found that the double-excitation cross sections are sensitive to the sign of the projectile charge, but that the energy region where this sensitivity is of the same order as for double ionization is 0.1 to 0.5 MeV/amu, whereas the latter has peak charge sensitivity at 1.5 MeV/amu. Comparison is made with some experimental results.

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I. INTRODUCTION

Describing reactions involving more than one electron requires information about the dynamics of few-electron phenomena, i.e., information required to describe how relatively complex many-body systems change. Since cross sections for two-electron transitions involve comparatively simple few-electron processes, various studies of two-electron transition cross sections have been undertaken [1–10,12,13]. In this paper we present a theoretical technique for calculating cross sections that is applicable to such multielectron processes, and thus may be used to comprehensively probe the dynamics of multielectron effects at reduced computational cost. Here we detail one method that has been used [1] to describe and evaluate cross sections for two-electron transitions in atoms which interact with fast bare projectiles of charge Z_p. This method uses a Born expansion in the projectile interaction strength Z_p and incorporates all terms in the electron-electron interaction. The leading term in Z_p is reduced to a closed analytic form. The second-order term is expressed as a one-dimensional energy integral over a product of two off-energy-shell first-order amplitudes, and so on. The technique is illustrated here for double excitation of helium.

Within the last decade, observations of double ionization in helium by protons [2], electrons [3], positrons [4], and antiprotons [5] have led to various calculations and interpretations [6]. In particular, the ratio of double– to single-ionization cross sections for helium is larger by a factor of 2 for positively charged projectiles than it is for

negatively charged projectiles in the energy region around 1.5 MeV/amu. Pedersen and Folkmann [9] and Fuelling et al. [10] have observed a difference of this order for excitation-ionization of helium by proton and electron projectiles at 1 to 4 MeV/amu. Also, a non-Z_p^2 dependence of the double excitation of helium has been reported by Pedersen and Hvelplund [11] and by Giese et al. [13]. The charge sensitivity of atomic scattering cross sections has been a useful probe of the underlying physics since the observations in 1956 by Barkas, Birnbaum, and Smith [14] of Z_p^3 effects in single ionization and excitation by positive and negative pion projectiles.

The first calculations of two-electron transition cross sections were done by Reading and Ford [7] using the forced impulse method (FIM), in which the system interacts in a series of sudden impulses with the projectile, evolving with a fully correlated propagator between impulses. A second-order FIM calculation, as used by Reading and Ford, is similar to our method, although different expansions for correlated electronic wave functions may be used. More recently, a variety of authors have used close-coupling calculations [15–17] to evaluate cross sections for double excitation. Here different numbers of iterations in the projectile interaction may be used and correlated wave functions may be employed. Recently, Ishihara [18] has used the technique of many-body perturbation theory (MBPT) to evaluate cross sections. The MBPT approach truncates expansions in both the projectile interaction and the electron correlation interaction. Bachau et al. [19] have developed calculations through first order in Z_p and all orders in the correlation interaction. Both calculations of Ishihara and Bachau

et al. include interference of the double-excitation resonance with the single-ionization background which is omitted in the other calculations of double excitation.

II. FIRST-ORDER TERM

The probability amplitude for transition from an initial state $|i\rangle$ to a final state $\langle f|$ may be written as [8,12]

$$a_{if} = \left\langle f \left| T \exp\left[-i \int V(t)dt\right] \right| i \right\rangle , \tag{1}$$

where T is the time-ordering operator [20], and V is the interaction between the projectile and the j electrons in the atom, namely,

$$V(t) = \sum_j e^{iH_0 t} V_j(t) e^{-iH_0 t} \tag{2}$$

with

$$V_j(t) = -\frac{Z_p}{|\mathbf{R}(t) - \mathbf{r}_j|} + \frac{Z_p}{R} . \tag{3}$$

The second term in (3) is required to cancel the monopole term in $Z_p/|\mathbf{R}(t) - \mathbf{r}_j|$ that would otherwise lead to a divergent term in (9) as ω goes to zero. Physically we have paired each target electron with a proton in the target nucleus so that all long-range Coulomb phases (which for neutral targets are entirely absent in our formulation) are carried by the internuclear terms [21]. The Born expansion of the amplitude is then given by

$$a_{fi} = a_{fi}^{(0)} + a_{fi}^{(1)} + a_{fi}^{(2)} + \cdots , \tag{4}$$

where $a_{fi}^{(0)} = \langle f|i\rangle$, which will be zero for the problems under consideration. For helium, the first-order amplitude is

$$a_{fi}^{(1)} = -i \int_{-\infty}^{\infty} dt \, \langle f| e^{iH_0 t} [V_1(t) + V_2(t)] e^{-iH_0 t} |i\rangle . \tag{5}$$

For the initial and final states, it is shown herein that

approximate two-electron wave functions consisting of a weighted product of one-electron wave functions, with the coefficients chosen by diagonalizing the fully correlated two-electron Hamiltonian, facilitate the reduction of amplitudes to the minimal number of dimensions requiring numerical integration (0 and 1 for first- and second-order amplitudes, respectively). This is because the difficult electron-electron interaction integrals are sequestered from (may be calculated in a separate computer code from) the scattering amplitude integrals. The contribution of these electron correlation terms is included within the numerical weighting factors $C_{\mu\nu}$ of the one-electron pair-product terms in the configuration-interaction (CI) wave functions. In the case of helium, these are

$$|i\rangle = \sum_{\alpha_i, \alpha_2} C_{\alpha_1 \alpha_2} |\alpha_1\rangle |\alpha_2\rangle$$

$$= 0.09916|1s\rangle|1s\rangle - 0.1251|1s\rangle|2s\rangle$$

$$- 0.0230|2s|2s\rangle + 0.0251|2p\rangle|2p\rangle \tag{6}$$

and (for the $2s^2 \, {}^1S$ final state)

$$\langle f| = \sum_{\beta_1, \beta_2} \overline{C}_{\beta_1 \beta_2} \langle \beta_1| \langle \beta_2|$$

$$= 0.8796\langle 2s|\langle 2s| + 0.4756\langle 2p|\langle 2p| . \tag{7}$$

Here $\langle nl|\langle nl'|$ are coupled to a well-defined angular momentum (e.g., ${}^1S$). In finding the CI wave functions, one has the freedom to choose the effective charge on the target nucleus. The choice $Z_{\text{eff}} = \lambda = 1.76$ minimized the ground-state energy (1% error) and nearly minimizes the excited-state energies. To avoid orthogonality problems, this value was used for both the initial and final states. The wave functions for the $2p^2 \, {}^1S^e$, $2s2p \, {}^1P^o$, and $2p^2 \, {}^1D^e$ final states are given in Appendix A.

Use of (6) and (7) gives for the fully correlated two-electron amplitude (5)

$$a_{2s^2,1s^2}^{(1)}(\omega) = -i\{2\overline{C}_{2s^2} C_{1s^2} A_{2s,1s}^{\lambda'\lambda}(\omega)\langle 2s\lambda'|1s\lambda\rangle + \sqrt{2}\overline{C}_{2s^2} C_{1s2s}[A_{2s,1s}^{\lambda'\lambda}(\omega)\langle 2s\lambda'|2s\lambda\rangle + A_{2s,2s}^{\lambda'\lambda}(\omega)\langle 2s\lambda'|1s\lambda\rangle]$$

$$+ 2\overline{C}_{2s^2} C_{2s^2} A_{2s,2s}^{\lambda'\lambda}(\omega)\langle 2s\lambda'|2s\lambda\rangle + \tfrac{2}{3}\overline{C}_{2p^2} C_{2p^2}[A_{210,210}^{\lambda'\lambda}(\omega)\langle 2p\lambda'|2p\lambda\rangle + 2A_{211,211}^{\lambda'\lambda}(\omega)\langle 2p\lambda'|2p\lambda\rangle]\} , \tag{8}$$

consisting of a weighted sum of pair products of one-electron scattering amplitudes,

$$A_{n'l'm',nlm}^{\lambda'\lambda}(\omega) = \int_{-\infty}^{\infty} dt \, e^{i\omega t} \left\langle n'l'm'\lambda' \left| \frac{-Z_p}{|\mathbf{R}(t) - \mathbf{r}|} + \frac{Z_p}{R} \right| nlm\lambda \right\rangle , \tag{9}$$

and (angular plus radial) overlap integrals $\langle n'l'm'\lambda'|nlm\lambda\rangle$. The parameters $\lambda = Z_t/a_0$ and $\lambda' = Z_t'/a_0$ allow for a change in screening between initial and final states, respectively.

Without correlation (if only $C_{1s1s} \neq 0$) the first-order term is zero, which implies that there would be no quantum interference leading to a Z_p^3 dependence in the cross section. The transition amplitudes to the other three final states are given in Appendix A.

For a straight-line projectile trajectory, a typical one-electron transition amplitude is [22]

$$A^{\lambda\lambda}_{2s,1s}(\omega)=\int_{-\infty}^{\infty}dt\,e^{i\omega t}\int d^3r\,u^{\lambda*}_{2s}(\mathbf{r})\left[\frac{-Z_p}{|\mathbf{R}(t)-\mathbf{r}|}\right.$$

$$\left.+\frac{Z_p}{R}\right]u^{\lambda}_{1s}(\mathbf{r})$$

$$=\frac{-Z_p\sqrt{2}\lambda^4 B}{v_p A^2}K_2(BA)\;,\tag{10}$$

where $A=[(\omega/v)^2+(3\lambda/2)^2]^{1/2}$, $\lambda=Z_t/a_0$, $\omega=E_f-E_i$, v_p is the projectile velocity, B is the impact parameter, and K_2 is a modified Bessel function of the second kind. The full set of one-electron transition amplitudes of the $n=1,2$ manifold is given in Appendix B. Straton has derived [23] an analytic form for the general one-electron state-to-state transition amplitude (9). Thus the first-order amplitude for double excitation (multiple excitation for many-electron atoms) may be given in closed analytic form to arbitrary precision simply by adding in more CI terms.

For final states such as double ionization, satisfying three-body Coulomb boundary conditions, one may use one-electron pseudostates [24] instead of the hydrogenic states and, again, introduce the electronic correlation in the CI weighting coefficients. Because one-electron pseudostates have the same analytic form as hydrogenic orbitals, application of comprehensive reduction techniques [23] will again yield an analytic first-order amplitude to arbitrary precision. One may instead use Coulomb-wave states written as a one-dimensional integral of an imaginary exponential that may also be integrated using Straton's technique [25], yielding amplitudes of the present form, but integrated over an additional dimension for each such state.

III. SECOND-ORDER TERM

The second-order amplitude is

$$a^{(2)}_{fi}=(-i)^2\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'\frac{T}{2}\langle f|e^{iH_0 t}[V_1(t)+V_2(t)]e^{-iH_0(t-t')}[V_1(t')+V_2(t')]e^{-iH_0 t'}|i\rangle\;,\tag{11}$$

where T is the time-ordering operator. If one were to neglect all correlations and set $T\equiv 1$, then (11) would reduce to the independent-electron approximation [26].

The asymptotic states are correlated because of (6) and (7), and one may likewise put correlation into the scattering region (scattering propagator) by inserting a complete set of correlated (CI) intermediate states:

$$\langle n|=\sum_{v_1,v_2}\hat{C}_{v_1 v_2}\langle v_1|\langle v_2|\;.\tag{12}$$

Even with this propagator, (11) is still not in a form that will allow integrations akin to (9). But if the time-ordered intermediate-state propagator is replaced by its integral representation [27],

$$\frac{T}{2}e^{-iE_n(t-t')}=\Theta(t-t')e^{-iE_n(t-t')}$$

$$=\frac{i}{2\pi}\int_{-\infty}^{\infty}d\Omega\frac{e^{-i\Omega(t-t')}}{\Omega-E_n+i\eta}$$

$$=\int_{-\infty}^{\infty}d\Omega\,e^{-i\Omega(t-t')}\left[\frac{1}{2}\delta(\Omega-E_n)+\frac{i}{2\pi}P\frac{1}{\Omega-E_n}\right]\;,\tag{13}$$

this casts all time dependence into the Ω exponential, giving time integrals of the same form as for the first-order amplitude. Thus the exact second-order amplitude may be reduced to

$$a_{fi}^{(2)} = \sum\!\!\!\!\!\!\int_n \sum_{\beta_1,\beta_2} \bar{C}_{\beta_1,\beta_2} \sum_{\alpha_1,\alpha_2} C_{\alpha_1,\alpha_2}$$

$$\times \left\{ \frac{(-i)^2}{2} \left[\sum_{\nu_1} \sum_{\nu_2'} \hat{C}_{\nu_1,\beta_2} \hat{C}_{\alpha_1,\nu_2'} A_{\beta_1,\nu_1}^{\lambda'\lambda}(E_f - E_n) A_{\nu_2',\alpha_2}^{\lambda'\lambda}(E_n - E_i) \right.\right.$$

$$\left. + \sum_{\nu_2} \sum_{\nu_1'} \hat{C}_{\beta_1,\nu_2} \hat{C}_{\nu_1',\alpha_2} A_{\beta_2,\nu_2}^{\lambda'\lambda}(E_f - E_n) A_{\nu_1',\alpha_1}^{\lambda'\lambda}(E_n - E_i) \right]$$

$$- \frac{i}{2\pi} P \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega - E_n} \left[\sum_{\nu_1} \sum_{\nu_2'} \hat{C}_{\nu_1,\beta_2} \hat{C}_{\alpha_1,\nu_2'} A_{\beta_1,\nu_1}^{\lambda'\lambda}(E_f - \Omega) A_{\nu_2',\alpha_2}(\Omega - E_i) \right.$$

$$\left.\left. + \sum_{\nu_2} \sum_{\nu_1'} \hat{C}_{\beta_1,\nu_2} \hat{C}_{\nu_1',\alpha_2} A_{\beta_2,\nu_2}^{\lambda'\lambda}(E_f - \Omega) A_{\nu_1',\alpha_1}^{\lambda'\lambda}(\Omega - E_i) \right] \right\} , \qquad (14)$$

where $\sum\!\!\!\!\!\int_n$ extends over the bound and continuum intermediate states and $A_{\beta\alpha}(E)$ is the one-electron transition matrix element (9). Here terms quadratic in V_1 or V_2 are omitted because they correspond to third- or (higher-) order amplitudes in the sense that they go to zero when the electron-electron interaction is removed. That is, we retain only the V_1V_2 and V_2V_1 contributions in (11). The amplitudes for all four final states are given explicitly in Appendix C.

The closure approximation may be used at this point to remove the infinite sum over intermediate states. This is done by approximating E_n for each of the intermediate states $|n\rangle$ by a common average energy $\bar{E}$. Then the propagator over intermediate states, i.e., (13), becomes independent of n and one may apply the closure relation $\sum_n |n\rangle\langle n| = 1$ when substituting (12) and (13) into (11). The second-order amplitude using the closure approximation then becomes

$$a_{fi}^{(2)} = \sum_{\beta_1,\beta_2} \bar{C}_{\beta_1,\beta_2} \sum_{\alpha_1,\alpha_2} C_{\alpha_1,\alpha_2} \left\{ \frac{(-i)^2}{2} [A_{\beta_1,\alpha_1}^{\lambda'\lambda}(E_f - \bar{E}) A_{\beta_2,\alpha_2}^{\lambda'\lambda}(\bar{E} - E_i) + A_{\beta_2,\alpha_2}^{\lambda'\lambda}(E_f - \bar{E}) A_{\beta_1,\alpha_1}^{\lambda'\lambda}(\bar{E} - E_i)] \right.$$

$$- \frac{i}{2\pi} P \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega - \bar{E}} [A_{\beta_1,\alpha_1}^{\lambda'\lambda}(E_f - \Omega) A_{\beta_2,\alpha_2}^{\lambda'\lambda}(\Omega - E_i)$$

$$\left. + A_{\beta_2,\alpha_2}^{\lambda'\lambda}(E_f - \Omega) A_{\beta_1,\alpha_1}^{\lambda'\lambda}(\Omega - E_i)] \right\} . \qquad (15)$$

This closure approximation avoids the infinite sum over intermediate states, $|n\rangle$. We note the principal-value part of (15) may be shown algebraically to be zero at $\bar{E} = (E_i + E_f)/2$ for $\lambda = \lambda'$.

The first group of terms in the exact second-order amplitude of (14) are known analytical functions. The second group consists of a principle-value integral of the first group. This principal-value term is nonzero when the energy variable Ω differs from the energy E_n of the intermediate state, corresponding to energy nonconserving contributions about E_n. If these principal-value contributions are ignored one obtains the results of Stotler-foht [28] where the imaginary terms are not present. As with second-order calculations of the Thomas peak [29] the real and imaginary parts of the present second-order amplitude obey a dispersion relation. It is possible that the principle-value integral may be evaluated analytically using Hilbert transforms [30] of Meijer's generalized hypergeometric functions. In any case, that one may reduce the second-order amplitude to an analytic part

plus a one-dimension integral shows the utility of CI wave functions and of the integrodifferential transform developed to evaluate the one-electron amplitudes in general [23].

The exact transition amplitude through second order may thus be expressed [1] as

$$a = -i(c_1 - c_2 Z_p) Z_p - \bar{c}_2 Z_p^2 , \qquad (16)$$

where c_1 is the first-order contribution, c_2 is the principal-value second-order contribution from (14), and $\bar{c}_2$ is the real part of the second-order contribution of (14). Hence, the cross section is

$$\sigma = \int |a|^2 d^2B = C_1^2 Z_p^2 - 2C_{12} Z_p^3 + \bar{C}_2^2 Z_p^4 + C_2^2 Z_p^4 . \qquad (17)$$

Then the difference of cross sections for excitation by protons and antiprotons is

$$\sigma(-) - \sigma(+) = 4C_{12} Z_p^3 . \qquad (18)$$

Thus, any Z_p^3 contribution to the experimentally mea-

sured cross section is evidence of both time ordering (C_2) and its consequent energy nonconserving contributions, and spatial correlation (C_1).

IV. RESULTS

The second-order amplitude (15) for double excitation of helium was evaluated in the closure approximation. It is conventional [31] to choose the "average energy" $\bar{E}$ at the ionization threshold. In the present case there are two such thresholds at 24.5876 and 79.0059 eV above the helium ground state. We choose our "average energy" to be midway between these two at 51.7965 eV above the helium ground state. This choice has an advantage of lying well below the series of doubly excited states beginning at 57.87 eV above the ground state. As $\bar{E}$ was varied from 20.616 to 79.0059 eV our cross sections generally varied by less than about 10%, except, of course, at $\bar{E} = E_f$ where resonances occur in (15) and cross sections increase by up to a factor of 5. The choice of $\bar{E}$ = 51.7965 eV used for the cross sections presented in this paper is further supported by noting that singly ionized states within this energy region play a major role in the experimental observations [13] so their contributions to intermediate states are well established. Even with the closure approximation, our present results go two steps beyond an independent-electron approximation through the inclusion of correlation and time ordering.

Figure 1 shows the present results plotted for proton and antiproton impact excitation of helium into the $2p^2\,{}^1D^e$ final state as a function of projectile energy. Also shown is the experimental measurement of Giese et al. [13] and the close-coupling calculations of Fritsch and Lin [15] for protons and electrons at 1.5 MeV/amu. Even though the first- and second-order (or IEA) cross sections are of equivalent magnitude over the entire ener-
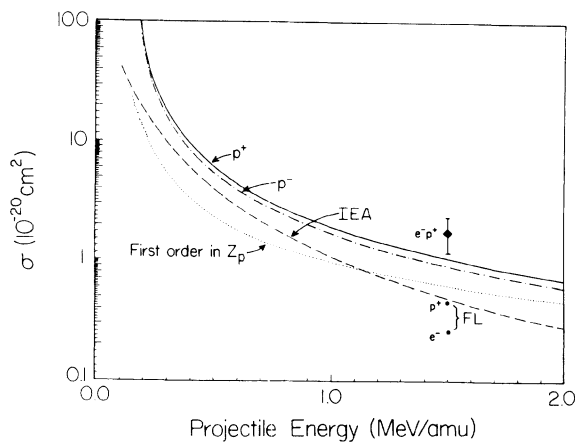
gy range from 0.1 to 2 MeV/amu, the interference between the two is only of order 10%, as seen by the $p - \bar{p}$ differences. In contrast, the close-coupling calculation [15] gave a difference of a factor of 2 between cross sections for protons and antiprotons. The error bars on the experimental data are large enough that one can draw no conclusions in support of either prediction. As for the magnitude of the results, the present calculation lies just below the data and lies higher than the result of Fritsch and Lin by a factor of 2 (3) for protons (antiprotons).

Figure 2 shows the cross sections for excitation into the $2s2p\,{}^1P^o$ final state. In addition to the data displayed in Fig. 1, Fig. 2 includes the experimental result of Pedersen and Hvelplund [11] at 1.84 MeV/amu. Although these data are the sum of their $2s2p\,{}^1P^o$ and $2p^2\,{}^1D^e$ cross sections, comparison with the present calculation is appropriate since the cross section for the latter final state is negligible compared to the former in the present theory. Again, the charge-sign effects in the experiments are masked by the error bars. In this case both the present calculation and that of Fritsch and Lin give a $p - \bar{p}$ difference of only order 10% at 1.5 MeV/amu. However, in the projectile impact energy region from 0.1 to 0.5 MeV/amu the present results give factor of 2 differences. This also holds true for excitation into the $2p^2\,{}^1S^e$ final state (not shown).

The present cross section for $2s2p\,{}^1P^o$ excitation lies higher than the calculation of Fritsch and Lin, which is larger than the experimental result of Giese et al. In Fig. 2 it is clear that the present cross section is almost exclusively first order near 1.5 MeV/amu. Fritsch and Lin note that their result is also dominated by the first-order matrix element [see their Eq. (7)]. Thus it is somewhat surprising that these two first-order calculations disagree and that they disagree with the data. For helium, disagreement with experiment may be because of interference of the doubly excited state that we evaluate with the single-ionization background that we do not include at this stage of our calculation. Also, since the
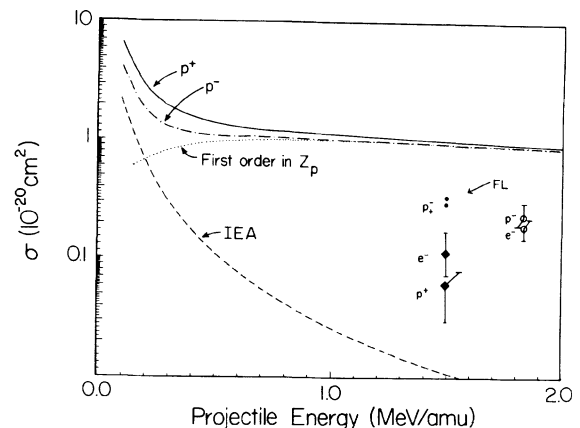

FIG. 1. Excitation of helium into the $2p^2\,{}^1D^e$ final state. The solid curve is the second-order theory for proton impact and the dash-dotted curve is for antiprotons. The dashed curve is the independent-electron approximation and the dotted curve is the first-order result. The data points for proton and electron impact are from Giese et al. (Ref. [13]) and the other two points at 1.5 MeV/amu are the close-coupling calculation of Fritsch and Lin (Ref. [15]).

FIG. 2. Excitation of helium into the $2s2p\,{}^1P^o$ final state. The curves are as in Fig. 1 with the addition of the observation of the sum of excitations into the $2p^2\,{}^1D^e$ and $2s2p\,{}^1P^o$ states at 1.84 MeV/amu by Pedersen and Hvelplund (Ref. [11]).
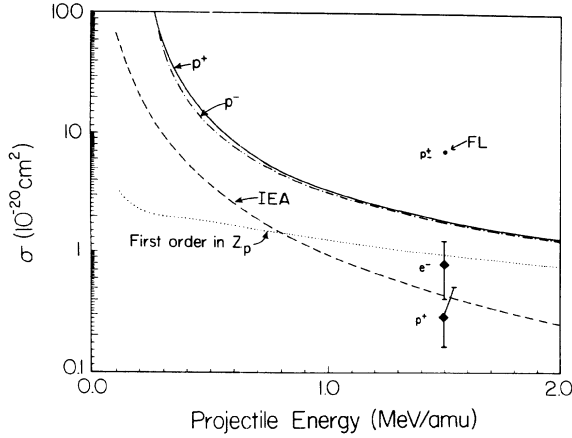
FIG. 3. Excitation of helium into the $2s^2\,{}^1S^e$ final state. The curves are as in Fig. 1. Winter's calculation (Ref. [17]) (not shown) lies slightly above the data at 1.5 MeV.

present first-order calculation is "exact" only to the degree that the initial and final wave functions accurately represent the helium atom, truncation of the series (6) and (7) is a possible source of error.

Alternatively, our result may lie higher because in using $Z_{\rm eff}=1.76$ as the effective charge for the doubly excited states (to keep the initial and final states orthogonal), we have included some portion of the continuum. The exact eigenstates of the Hamiltonian can be constructed as a linear combination of doubly excited states and the continuum states, in which the former are embedded. To calculate the wave function of the doubly excited part, one needs to project this Hamiltonian onto the bound states [32]. A general practice [33] is to use a basis set constructed of two one-electron eigenstates excluding all the states with one-electron energies below the doubly excited states. In our case, we could simply use $Z_{\rm eff}=2$ and choose the basis set $|n_1l_1,n_2l_2LM\rangle$ such that $n_1,n_2>1$. Either case indicates that experimental determinations of the $2s2p\,{}^1P^o$ excitation cross sections may provide a sensitive measure of the quality of approximate two-electron wave functions.

Figure 3 shows the cross section for excitation into the $2s^2\,{}^1S^e$ final state. In this case the independent-electron approximation, which contains only the $1s^2$ term in the initial-state wave function, and thus is uncorrelated, and contains no time-ordering effects, best represents the

data. This is likely to be a fortuitous canceling of effects. The result of Winter [17], who uses some continuum intermediate contributions, lies close to the observed results [13].

V. CONCLUSION

We have presented a technique for evaluating cross sections for double excitation of atoms by fast particles of charge Z_p. The amplitude first order in Z_p has been given in analytic form and may be made as exact as desired. The second-order amplitude contains an analytic energy-conserving term (correlated generalization of the IEA) and an energy-nonconserving (time-ordered) term that interferes with the first-order term. The energy-nonconserving term in the second-order amplitude is given by a one-dimensional integral over intermediate energies. This method may by applied to ionization-excitation and double ionization if appropriate pseudostates are used to describe continuum wave functions. This technique significantly reduces the computer costs of multielectron calculations. In actual calculations for double excitation of helium, ignoring background continuum states, differences in the cross sections for impact excitation by protons versus antiprotons have been found to be of order 10% at 1.5 MeV/amu.

APPENDIX A

The CI wave function used for the $2p^2\,{}^1S^e$ final state is

$$\langle 2p^2\,{}^1S^e| = 0.8796\langle 2p|\langle 2p| - 0.4756\langle 2s|\langle 2s| ,\qquad (A1)$$

for the $2s2p\,{}^1P^o$ final state is

$$\langle 2s2p\,{}^1P^o| = 1.0\langle 2s|\langle 2p| ,\qquad (A2)$$

and for the $2p^2\,{}^1D^e$ final state is

$$\langle 2p^2\,{}^1D^e| = 1.0\langle 2p|\langle 2p| .\qquad (A3)$$

The first-order amplitude for excitation into the $2p^2\,{}^1S^e$ final state is identical to that for the $2s^2\,{}^1S^e$ except for the interchange of CI coefficients. The first-order amplitude for excitation into the $2s2p\,{}^1P^o$ final states is

$$a^{(1)}_{2s211,1s^2}(\omega) = -i\overline{C}_{2s2p}\left\{\frac{2}{\sqrt{2}}C_{1s^2}A^{\lambda'\lambda}_{211,1s}(\omega)\langle 2s\lambda'|1s\lambda\rangle + \frac{2}{\sqrt{2}}C_{2s^2}A^{\lambda'\lambda}_{211,2s}(\omega)\langle 2s\lambda'|2s\lambda\rangle\right.$$

$$+ C_{1s2s}[A^{\lambda'\lambda}_{211,1s}(\omega)\langle 2s\lambda'|2s\lambda\rangle + A^{\lambda'\lambda}_{211,2s}(\omega)\langle 2s\lambda'|1s\lambda\rangle]$$

$$\left. + \frac{2}{\sqrt{6}}C_{2p^2}A^{\lambda'\lambda}_{2s,21-1}(\omega)\langle 2p\lambda'|2p\lambda\rangle\right\}\qquad (A4)$$

for the $m=1$ sublevel and

$$a^{(1)}_{2s210,1s^2}(\omega) = -i\overline{C}_{2s2p}\left\{\frac{2}{\sqrt{2}}C_{1s^2}A^{\lambda'\lambda}_{210,1s}(\omega)\langle 2s\lambda'|1s\lambda\rangle + \frac{2}{\sqrt{2}}C_{2s^2}A^{\lambda'\lambda}_{210,2s}(\omega)\langle 2s\lambda'|2s\lambda\rangle\right.$$

$$+C_{1s2s}[A^{\lambda'\lambda}_{210,1s}(\omega)\langle 2s\lambda'|2s\lambda\rangle + A^{\lambda'\lambda}_{210,2s}(\omega)\langle 2s\lambda'|1s\lambda\rangle]$$

$$\left.+\frac{2}{\sqrt{6}}C_{2p^2}(-1)A^{\lambda'\lambda}_{2s,210}(\omega)\langle 2p|2p\rangle\right\}.\tag{A5}$$

For the $m=-1$ sublevel, the amplitude is the negative of (A4).

The first-order amplitude for excitation into the $2p^2\,{}^1D^e$ final state is

$$a^{(1)}_{2p^2\,{}^1D^e\,M=2,1s^2}(\omega) = -i\frac{2}{\sqrt{3}}\overline{C}_{2p^2}C_{2p^2}A^{\lambda'\lambda}_{211,21-1}(\omega)$$

$$\times\langle 2p\lambda'|2p\lambda\rangle\tag{A6}$$

for the $m=2$ sublevel,

$$a^{(1)}_{2p^2\,{}^1D^e\,M=1,1s^2}(\omega) = i\frac{2\sqrt{2}}{\sqrt{3}}\overline{C}_{2p^2}C_{2p^2}A^{\lambda'\lambda}_{211,210}(\omega)$$

$$\times\langle 2p\lambda'|2p\lambda\rangle\tag{A7}$$

for the $m=1$ sublevel, and

$$a^{(1)}_{2p^2\,{}^1D^e\,M=0,1s^2}(\omega) = -i\frac{2\sqrt{2}}{3}\overline{C}_{2p^2}C_{2p^2}$$

$$\times[A^{\lambda'\lambda}_{211,211}(\omega) - A^{\lambda'\lambda}_{210,210}(\omega)]$$

$$\times\langle 2p\lambda'|2p\lambda\rangle\tag{A8}$$

for the $m=0$ sublevel. For the $m=-1$ sublevel, the amplitude is the negative of (A7). For the $m=-2$ sublevel, the amplitude equals (A6).

APPENDIX B

The general one-electron state-to-state transition amplitude has been given by Straton [23] in closed analytic form. To accomplish this, Straton developed [34] an integrodifferential transform to replace the Fourier transform, because the latter becomes extremely awkward for integrating excited states since it results in a "final" expression containing derivatives of parameters rather than simple analytic functions. However, in individual cases these derivatives may be evaluated to obtain analytic functions. This was done for each of the following amplitudes to verify their accuracy.

The amplitudes for transitions from the ground state into the $n=2$ and 3 for $Z_t=1$ were first calculated by Van Den Bos and De Heer [22] and then Hopkins, Brenn, and Whittemore [35] scaled those results for higher values of the target charge Z_t. McAbee [36] calculated the $2p\leftarrow 1s$ transition amplitude in a case where there is a change of screening between initial and final states. McGuire et al. [37] found the $2p\leftarrow 2s$ amplitudes.

The following amplitudes are for completely general charges, allowing for a change of screening between initial and final states, through the initial- and final-state parameters $\lambda=Z_t/a_0$ and $\lambda'=Z_t'/a_0$, respectively. As noted by Straton [23], the amplitudes calculated by Van Den Bos and De Heer [22] contain an error in phase, arising from their use of the erroneous phase in the momentum-space hydrogenic wave function derived by Podolsky and Pauling [38]. The phase is given correctly in the following. In all expressions $A_{n'n}=(\alpha^2+\gamma^2_{n'n})^{1/2}$, $\gamma_{n'n}=\lambda'/n'+\lambda/n$, $\alpha=\omega/v_p$, $\omega=E_f-E_i$, v_p is the projectile velocity, B is the impact parameter, and K_ν is a modified Bessel function of the second kind.

The one-electron transition $n=1$ amplitude is

$$A^{\lambda'\lambda}_{1s,1s}(\omega) = \frac{16(\lambda'\lambda)^{3/2}Z_pZ_e}{\gamma^3_{11}v_p}\left[-K_0(BA_{11})\right.$$

$$\left.-\frac{\gamma^2_{11}B}{2A_{11}}K_1(BA_{11})\right].\tag{B1}$$

The one-electron transition $\{n',n\}=\{1,2\}$ mixed manifold amplitudes are

$$A^{\lambda'\lambda}_{2s,1s}(\omega) = A^{\lambda\lambda'}_{1s,2s}\{21\rightarrow 12\}(\omega)$$

$$=\frac{2\sqrt{2}(\lambda'\lambda)^{3/2}Z_pZ_e}{\gamma^3 v_p}\left\{(\lambda'-\lambda)\left[\frac{2}{\gamma}K_0(BA_{21})+\frac{\gamma B}{A_{21}}K_1(BA_{21})\right]\right.$$

$$\left.+\frac{\lambda'\gamma^3 B^2}{2A^2_{21}}\left[K_0(BA_{21})+\frac{2}{BA_{21}}K_1(BA_{21})\right]\right\},\tag{B2}$$

$$A^{\lambda'\lambda}_{210,1s}(\omega) = A^{\lambda\lambda'}_{1s,210}\{21\rightarrow 12\}(\omega)$$

$$=i\frac{\sqrt{2}\,8\lambda'^{5/2}\lambda^{3/2}Z_pZ_e}{\gamma^5 v_p}\alpha\left\{K_0(B\alpha)-\left[1+\frac{\gamma^4 B^2}{8A^2_{21}}\right]K_0(BA_{21})-\left[\frac{B\gamma^2}{2A_{21}}+\frac{\gamma^4 B}{4A^3_{21}}\right]K_1(BA_{21})\right\},\tag{B3}$$

and

$$A_{211,1s}^{\lambda'\lambda}(\omega) = -A_{21-1,1s}^{\lambda'\lambda}(\omega)$$

$$= A_{1s,211}^{\lambda\lambda'}\{21 \rightarrow 12\}(\omega)$$

$$= -A_{1s,21-1}^{\lambda\lambda'}\{21 \rightarrow 12\}(\omega)$$

$$= -\frac{8\lambda'^{5/2}\lambda^{3/2}Z_pZ_e}{\gamma_{21}^5 v_p}\left\{\alpha K_1(B\alpha) - \left[A_{21} + \frac{\gamma_{21}^4 B^2}{8A_{21}}\right]K_1(BA_{21}) - \frac{\gamma_{21}^2 B}{2}K_0(BA_{21})\right\}.$$ (B4)

The one-electron transition $\{n',n\} = \{2,2\}$ manifold amplitudes are, where $A = A_{22}$ and $\gamma = \gamma_{22}$,

$$A_{2s,2s}^{\lambda'\lambda}(\omega) = \frac{(\lambda'\lambda)^{3/2}Z_pZ_e}{\gamma^6 v_p}\left\{-\left[2(3\lambda'\lambda\gamma - 2\gamma^3) + \frac{\lambda'\lambda\gamma^7 B^2}{A^4} + (3\lambda'\lambda\gamma - 4\gamma^3)\frac{B^2\gamma^4}{4A^2}\right]K_0(BA_{22})\right.$$
$$\left. -\left[(3\lambda'\lambda\gamma - 2\gamma^3)\frac{\gamma^2 B}{A} + \frac{\lambda'\lambda\gamma^7}{4}\left[\frac{8B}{A^5} + \frac{B^3}{A^3}\right] + (3\lambda'\lambda\gamma - 4\gamma^3)\frac{B\gamma^4}{2A^3}\right]K_1(BA_{22})\right\},$$ (B5)

$$A_{210,2s}^{\lambda'\lambda}(\omega) = A_{2s,210}^{\lambda\lambda'}(\omega)$$

$$= i\frac{\lambda'^{5/2}\lambda^{3/2}Z_pZ_e}{\gamma^6 v_p}\alpha\left\{2(\lambda' - 4\lambda)K_0(B\alpha) - \left[(\lambda' - 4\lambda)\left[2 + \frac{\gamma^4 B^2}{4A^2}\right] - \frac{\lambda\gamma^6 B^2}{A^4}\right]K_0(BA_{22})\right.$$
$$\left. -\left[(\lambda' - 4\lambda)\left[\frac{B\gamma^2}{A} + \frac{\gamma^4 B}{2A^3}\right] - \frac{\lambda\gamma^6}{4}\left[\frac{8B}{A^5} + \frac{B^3}{A^3}\right]\right]K_1(BA_{22})\right\},$$ (B6)

$$A_{211,2s}^{\lambda'\lambda}(\omega) = -A_{21-1,2s}^{\lambda'\lambda}(\omega)$$

$$= A_{2s,211}^{\lambda\lambda'}(\omega)$$

$$= -A_{2s,21-1}^{\lambda\lambda'}(\omega)$$

$$= \frac{\lambda'^{5/2}\lambda^{3/2}Z_pZ_e}{\sqrt{2}\gamma^6 v_p}\left\{2(\lambda' - 4\lambda)\alpha K_1(B\alpha) - \left[(\lambda' - 4\lambda)\gamma^2 B - \frac{\lambda B^3\gamma^6}{4A^2}\right]K_0(BA_{22})\right.$$
$$\left. -\left[(\lambda' - 4\lambda)\left[2A + \frac{B^2\gamma^4}{4A}\right] - \frac{\lambda B^2\gamma^6}{2A^3}\right]K_1(BA_{22})\right\},$$ (B7)

$$A_{210,210}^{\lambda'\lambda}(\omega) = \frac{(\lambda'\lambda)^{5/2}Z_pZ_e}{\gamma^7 v_p}\left\{-\left[14\gamma^2 - \frac{3B^2\gamma^4}{2} + \frac{3\gamma^6 B^2}{4A^2} + \frac{\gamma^8 B^2}{A^4} - 12A^2\right]K_0(BA_{22})\right.$$
$$\left. -\left[\frac{4\gamma^4 B}{A} - \frac{B^3\gamma^6}{4A} + \frac{3\gamma^6 B}{2A^3} + \frac{2\gamma^8 B}{A^5} + \frac{\gamma^8 B^3}{4A^3} - 6B\gamma^2 A\right]K_1(BA_{22})\right\},$$ (B8)

$$A_{211,211}^{\lambda'\lambda}(\omega) = A_{21-1,21-1}^{\lambda'\lambda}(\omega)$$

$$= \frac{(\lambda'\lambda)^{5/2}Z_pZ_e}{\gamma^7 v_p}\left\{-[-4\gamma^2 + \tfrac{3}{4}\gamma^4 B^2 + 6A^2]K_0(BA_{22}) - \left[3\gamma^2 AB - \frac{\gamma^4 B}{2A} + \frac{\gamma^6 B^3}{8A}\right]K_1(BA_{22})\right\},$$ (B9)

and, since the following depend only on the product $\lambda'\lambda$,

$$A_{211,210}^{\lambda'\lambda}(\omega) = -A_{21-1,210}^{\lambda'\lambda}(\omega)$$

$$= A_{210,211}^{\lambda'\lambda}(\omega)$$

$$= -A_{210,21-1}^{\lambda'\lambda}(\omega)$$

$$= -i\frac{3\sqrt{2}(\lambda'\lambda)^{5/2}Z_pZ_e}{\gamma^7 v_p}$$

$$\times \alpha\left\{2|\alpha|K_1(B\alpha) - \left[\gamma^2 B + \frac{\gamma^6 B^3}{24A^2}\right]K_0(BA_{22}) - \left[2A + \frac{\gamma^4 B^2}{4A} + \frac{\gamma^6 B^2}{12A^3}\right]K_1(BA_{22})\right\}$$ (B10)

and

$$A^{\lambda'\lambda}_{211,21-1}(\omega) = A^{\lambda'\lambda}_{21-1,211}(\omega)$$

$$= -\frac{3(\lambda'\lambda)^{5/2}Z_pZ_e}{\gamma^7 v_p}\left\{2\alpha\left[\alpha K_0(B\alpha) + \frac{2}{B}K_1(B\alpha)\right] - \left[2A^2 + \frac{\gamma^4 B^2}{4}\right]K_0(BA_{22})\right.$$

$$\left. - \left[\frac{4A}{B} + \gamma^2 AB + \frac{\gamma^6 B^3}{24A}\right]K_1(BA_{22})\right\}. \tag{B11}$$

The relations

$$A^{\lambda'\lambda}_{n'l'm',nlm}(\omega B) = (-1)^{m'+m}A^{\lambda\lambda'}_{nl-m,n'l'-m'}(\omega B)$$

$$= (-1)^{m'+m}[A^{\lambda'\lambda}_{n'l'-m',nl-m}(-\omega B)]^* = [A^{\lambda\lambda'}_{nlm,n'l'm'}(-\omega B)]^* \tag{B12}$$

have been used to find the amplitudes with permuted parameters. In (9) we have set $Z_e = -1$.

APPENDIX C

The real parts of the second-order amplitudes are

$$\mathrm{Re}[a^{(2)}_{2s^2,1s^2}] = -\left\{\overline{C}_{2s^2}C_{1s^2}A^{\lambda'\lambda}_{2s,1s}(\omega_1)A^{\lambda'\lambda}_{2s,1s}(\omega_2)\right.$$

$$+\sqrt{2}\,\overline{C}_{2s^2}C_{1s2s}A^{\lambda'\lambda}_{2s,1s}(\omega_1)A^{\lambda'\lambda}_{2s,2s}(\omega_2) + \overline{C}_{2s^2}C_{2s^2}A^{\lambda'\lambda}_{2s,2s}(\omega_1)A^{\lambda'\lambda}_{2s,2s}(\omega_2)$$

$$+\frac{\overline{C}_{2s^2}C_{2p^2}}{\sqrt{3}}[-2A^{\lambda'\lambda}_{2s,211}(\omega_1)A^{\lambda'\lambda}_{2s,211}(\omega_2) - A^{\lambda'\lambda}_{2s,210}(\omega_1)A^{\lambda'\lambda}_{2s,210}(\omega_2)]$$

$$+\frac{\overline{C}_{2p^2}C_{1s^2}}{\sqrt{3}}[-2A^{\lambda'\lambda}_{211,1s}(\omega_1)A^{\lambda'\lambda}_{211,1s}(\omega_2) - A^{\lambda'\lambda}_{210,1s}(\omega_1)A^{\lambda'\lambda}_{210,1s}(\omega_2)]$$

$$+\frac{\overline{C}_{2p^2}C_{1s2s}\sqrt{2}}{\sqrt{3}}[-2A^{\lambda'\lambda}_{211,1s}(\omega_1)A^{\lambda'\lambda}_{211,2s}(\omega_2) - A^{\lambda'\lambda}_{210,1s}(\omega_1)A^{\lambda'\lambda}_{210,2s}(\omega_2)]$$

$$+\frac{\overline{C}_{2p^2}C_{2s^2}}{\sqrt{3}}[-2A^{\lambda'\lambda}_{211,2s}(\omega_1)A^{\lambda'\lambda}_{211,2s}(\omega_2) - A^{\lambda'\lambda}_{210,2s}(\omega_1)A^{\lambda'\lambda}_{210,2s}(\omega_2)]$$

$$+\frac{\overline{C}_{2p^2}C_{2p^2}}{3}[2A^{\lambda'\lambda}_{211,211}(\omega_1)A^{\lambda'\lambda}_{211,211}(\omega_2) + 4A^{\lambda'\lambda}_{211,210}(\omega_1)A^{\lambda'\lambda}_{211,210}(\omega_2)$$

$$\left. -2A^{\lambda'\lambda}_{211,21-1}(\omega_1)A^{\lambda'\lambda}_{211,21-1}(\omega_2) + A^{\lambda'\lambda}_{210,210}(\omega_1)A^{\lambda'\lambda}_{210,210}(\omega_2)]\right\}, \tag{C1}$$

$$\mathrm{Re}[a^{(2)}_{2s,211;1s^2}] = -\overline{C}_{2s2p}\sqrt{2}\left\{C_{1s^2}A^{\lambda'\lambda}_{2s,1s}(\omega_1)A^{\lambda'\lambda}_{211,1s}(\omega_2) + \frac{C_{1s2s}}{\sqrt{2}}[A^{\lambda'\lambda}_{2s,1s}(\omega_1)A^{\lambda'\lambda}_{211,2s}(\omega_2) + A^{\lambda'\lambda}_{2s,2s}(\omega_1)A^{\lambda'\lambda}_{211,1s}(\omega_2)]\right.$$

$$+C_{2s^2}A^{\lambda'\lambda}_{2s,2s}(\omega_1)A^{\lambda'\lambda}_{211,2s}(\omega_2)$$

$$+\frac{C_{2p^2}}{\sqrt{3}}[-A^{\lambda'\lambda}_{2s,211}(\omega_1)A^{\lambda'\lambda}_{211,211}(\omega_2) - A^{\lambda'\lambda}_{2s,210}(\omega_1)A^{\lambda'\lambda}_{211,210}(\omega_2)$$

$$\left. +A^{\lambda'\lambda}_{2s,211}(\omega_1)A^{\lambda'\lambda}_{211,21-1}(\omega_2)]\right\}, \tag{C2}$$

$$\text{Re}[a^{(2)}_{2s,210;1s^2}] = -\bar{C}_{2s2p}\sqrt{2}\left\{ C_{1s^2} A^{\lambda'\lambda}_{2s,1s}(\omega_1)A^{\lambda'\lambda}_{210,1s}(\omega_2) + \frac{C_{1s2s}}{\sqrt{2}}[A^{\lambda'\lambda}_{2s,1s}(\omega_1)A^{\lambda'\lambda}_{210,2s}(\omega_2) + A^{\lambda'\lambda}_{2s,2s}(\omega_1)A^{\lambda'\lambda}_{210,1s}(\omega_2)]\right.$$

$$+ C_{2s^2} A^{\lambda'\lambda}_{2s,2s}(\omega_1)A^{\lambda'\lambda}_{210,2s}(\omega_2)$$

$$+ \frac{C_{2p^2}}{\sqrt{3}}[-A^{\lambda'\lambda}_{2s,211}(\omega_1)A^{\lambda'\lambda}_{211,210}(\omega_2) - A^{\lambda'\lambda}_{2s,210}(\omega_1)A^{\lambda'\lambda}_{210,210}(\omega_2)$$

$$\left. -A^{\lambda'\lambda}_{2s,211}(\omega_1)A^{\lambda'\lambda}_{211,210}(\omega_2)]\right\}, \tag{C3}$$

$$\text{Re}[a^{(2)}_{2p^2\,^1D^e,M=2,1s^2}] = -\bar{C}_{2p^2}\left\{ C_{1s^2} A^{\lambda'\lambda}_{211,1s}(\omega_1)A^{\lambda'\lambda}_{211,1s}(\omega_2)\right.$$

$$+\sqrt{2}C_{1s2s} A^{\lambda'\lambda}_{211,1s}(\omega_1)A^{\lambda'\lambda}_{211,2s}(\omega_2) + C_{2s^2} A^{\lambda'\lambda}_{211,2s}(\omega_1)A_{211,2s^{\lambda'\lambda}}(\omega_2)$$

$$\left. +\frac{C_{2p^2}}{\sqrt{3}}[2A^{\lambda'\lambda}_{211,21-1}(\omega_1)A^{\lambda'\lambda}_{211,211}(\omega_2) - A^{\lambda'\lambda}_{211,210}(\omega_1)A^{\lambda'\lambda}_{211,210}(\omega_2)]\right\}, \tag{C4}$$

$$\text{Re}[a^{(2)}_{2p^2\,^1D^e,M=1,1s^2}] = -\bar{C}_{2p^2}\sqrt{2}\left\{ C_{1s^2} A^{\lambda'\lambda}_{211,1s}(\omega_1)A^{\lambda'\lambda}_{210,1s}(\omega_2)\right.$$

$$+\frac{C_{1s2s}}{\sqrt{2}}[A^{\lambda'\lambda}_{211,1s}(\omega_1)A^{\lambda'\lambda}_{210,2s}(\omega_2) + A^{\lambda'\lambda}_{211,2s}(\omega_1)A^{\lambda'\lambda}_{210,1s}(\omega_2)]$$

$$+C_{2s^2} A^{\lambda'\lambda}_{211,2s}(\omega_1)A^{\lambda'\lambda}_{210,2s}(\omega_2)$$

$$+\frac{C_{2p^2}}{\sqrt{3}}[A^{\lambda'\lambda}_{211,21-1}(\omega_1)A^{\lambda'\lambda}_{211,210}(\omega_2) - A^{\lambda'\lambda}_{211,210}(\omega_1)A^{\lambda'\lambda}_{210,210}(\omega_2)$$

$$\left. -A^{\lambda'\lambda}_{211,211}(\omega_1)A^{\lambda'\lambda}_{211,210}(\omega_2)]\right\}, \tag{C5}$$

and

$$\text{Re}[a^{(2)}_{2p^2\,^1D^e,M=0,1s^2}] = -\frac{\bar{C}_{2p^2}\sqrt{2}}{\sqrt{3}}\left\{ C_{1s^2}[-A^{\lambda'\lambda}_{211,1s}(\omega_1)A^{\lambda'\lambda}_{211,1s}(\omega_2) + A^{\lambda'\lambda}_{210,1s}(\omega_1)A^{\lambda'\lambda}_{210,1s}(\omega_2)]\right.$$

$$+\sqrt{2}C_{1s2s}[-A^{\lambda'\lambda}_{211,1s}(\omega_1)A^{\lambda'\lambda}_{211,2s}(\omega_2) + A^{\lambda'\lambda}_{210,1s}(\omega_1)A^{\lambda'\lambda}_{210,2s}(\omega_2)]$$

$$+C_{2s^2}[-A^{\lambda'\lambda}_{211,2s}(\omega_1)A^{\lambda'\lambda}_{211,2s}(\omega_2) + A^{\lambda'\lambda}_{210,2s}(\omega_1)A^{\lambda'\lambda}_{210,2s}(\omega_2)]$$

$$+\frac{C_{2p^2}}{\sqrt{3}}[A^{\lambda'\lambda}_{211,21-1}(\omega_1)A^{\lambda'\lambda}_{211,21-1}(\omega_2) - A^{\lambda'\lambda}_{211,210}(\omega_2)A^{\lambda'\lambda}_{211,210}(\omega_2)$$

$$\left. -A^{\lambda'\lambda}_{210,210}(\omega_1)A^{\lambda'\lambda}_{210,210}(\omega_2) + A^{\lambda'\lambda}_{211,211}(\omega_1)A^{\lambda'\lambda}_{211,211}(\omega_2)]\right\}. \tag{C6}$$

For the $M = -1$ sublevel, the amplitudes are the negatives of (C2) and (C5). For the $M = -2$ sublevel, the amplitude equals (C4). The amplitude for $2p^2\,^1S^e$ is given by (C1), but with the CI coefficients interchanged as in (7) vs (A1).

The imaginary parts of the amplitudes are given by

$$\text{Im}[a^{(2)}(E_f,E_n,E_i)] = \frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{d\Omega}{\Omega-E_n}\text{Re}[a^{(2)}E_f,\Omega,E_i)]. \tag{C7}$$

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